Finite thermal conductivity in 1d lattices

C. Giardiná[1,2], R. Livi[3,4], A. Politi[5,4], and M. Vassalli[3]

[1] *Dipartimento di Fisica, via Irnerio 46, 40126 Bologna Italy*
[2] *Istituto Nazionale di Fisica Nucleare, Sez. di Bologna,*
[3] *Dipartimento di Fisica, L.go E. Fermi 2, 50125 Firenze, Italy*
[4] *Istituto Nazionale di Fisica della Materia, Unità di Firenze,*
[5] *Istituto Nazionale di Ottica, L.go E. Fermi 6, 50125 Firenze, Italy*

(February 5, 2008)

We discuss the thermal conductivity of a chain of coupled rotators, showing that it is the first example of a 1d nonlinear lattice exhibiting normal transport properties in the absence of an on-site potential. Numerical estimates obtained by simulating a chain in contact with two thermal baths at different temperatures are found to be consistent with those ones based on linear response theory. The dynamics of the Fourier modes provides direct evidence of energy diffusion. The finiteness of the conductivity is traced back to the occurrence of phase-jumps. Our conclusions are confirmed by the analysis of two variants of this model.

PACS numbers:

The understanding of heat conduction in insulating solids is a long-standing problem even in the simple context of 1d systems. Rigorous studies have shown that the thermal conductivity κ diverges (in the thermodynamic limit) in homogeneous [1] and disordered [2] harmonic chains. Accordingly, it has become transparent that the nonlinear character of the microscopic dynamics is a necessary ingredient for the emergence of the Fourier heat conduction law at the macroscopic level.

The typical Hamiltonians chosen to study this problem belong to the general class

$$H = \sum_{i=1}^{N} \left[\frac{p_i^2}{2m_i} + V(q_{i+1} - q_i) + U(q_i) \right], \qquad (1)$$

where m_i represents the mass of the i-th particle [3], V is the potential energy of internal forces and U is an on-site potential representing interactions with a possible external substrate.

The first convincing numerical evidence of a finite conductivity has been provided by the preliminary study of the ding-a-ling model [4] and the successive detailed analysis of the modified ding-dong model [5]. Such results have supported the conjecture that a strong chaotic dynamics is the crucial requisite for the observation of normal transport properties in 1d chains. *A fortiori*, this has been assumed to hold in higher-dimensions, where scattering effects, due to nonlinear interactions among normal modes, should make the diffusion process, at the basis of standard transport phenomena, even more efficient than in 1d systems.

However, the recent study of the more realistic FPU β-model ($V(x) = x^2/2 + x^4/4$, $U = 0$) has revealed a power-law divergence of the thermal conductivity as $\kappa \sim N^{2/5}$ [6] (where N is the chain length [7]). Such an anamalous behaviour has been explained by invoking the self-consistent mode coupling theory [8] in the description of the effective evolution of long-wavelength modes [9]. The generality of this result has been confirmed by the study of several models with no on-site potential, including the diatomic Toda model [10] that was previously believed to yield a finite conductivity. On the other hand, numerical results have accumulated indicating that whenever an external force is added (as in the above mentioned ding-a-ling and ding-dong models), the conductivity is finite [11]. As a consequence, it has been suggested that momentum conservation is the key ingredient responsible for an anomalous transport even in the presence of a chaotic evolution.

Such a conjecture has been very recently put on more firm grounds by Prosen and Campbell [12], who have shown that anomalous transport necessarily arises whenever two conditions are fulfilled: (*i*) the momentum is conserved; (*ii*) the pressure does not vanish in the thermodynamic limit. On the other hand, systems with symmetric potentials, such as the FPU-β model, do not belong to this class, since the pressure vanishes. In practice, as all momentum-conserving models studied in the literature have revealed anomalous transport properties, the possibility that the condition on the pressure is redundant remains open.

In this Letter, we show that this is not the case by analysing some 1d models where momentum is conserved and yet the conductivity is finite.

A. The rotator model The simplest example of a classical-spin 1d model with nearest neighbour interactions lies in the class (1) with $V(x) = 1 - \cos(x)$ and $U = 0$. This model can be read also as a chain of N coupled pendula, where the p_i's and the q_i's represent action-angle variables, respectively. It has been extensively studied [13,14] as an example of chaotic dynamical system [15] that becomes integrable both in the small and high energy limits, when it reduces to a harmonic chain and free-rotators, respectively. In the two inte-

grable limits, the relaxation to equilibrium slows down very rapidly for most of the observables of thermodynamic interest (e.g., the specific heat) [14]. As as consequence, the equivalence between ensemble and time averages is established over accessible time scales only inside a limited interval of the energy density ε. Here we shall discuss heat conduction for values of the energy density corresponding to strongly chaotic behaviour.

B. Numerical analysis of the thermal conductivity The most natural and direct way to determine κ consists in simulating a real experiment, by coupling the left and right extrema of the chain with two thermal baths at temperatures $T_L > T_R$, respectively. In our simulations we have used Nosé-Hoover models of thermostats [16], both because they can be easily implemented (integrating the resulting equations with a standard algorithm) and because of the smaller finite-size effects (due to the unavoidable contact resistance).

With this setting, a non-equilibrium stationary state sets in characterized by a non-vanishing heat flux J [17,6]:

$$J \;=\; \frac{1}{N}\sum_i j_i \;=\; \frac{1}{N}\sum_i \frac{p_i}{2}\,(f_{i+1}+f_i) \qquad (2)$$

where $f_i = -\partial V(q_{i+1}-q_i)/\partial q_i = \sin(q_{i+1}-q_i)$ is the interaction force and j_i is the local flux at site i. The total heat flux J has to be averaged over a sufficiently long time span to get rid of fluctuations and to ensure the convergence to the stationary regime. This can be tested by monitoring the average heat flux and looking at the scale of its fluctuations. As a result, we have verified that $2\cdot 10^6$ time units are sufficient to guarantee a few percents of fluctuations in the worst cases.

The thermal conductivity is determined by assuming the Fourier law, i.e. from the relation $J = \kappa \nabla T$, where ∇T denotes the imposed thermal gradient. The simulations have been performed for $T_L = 0.55$, $T_R = 0.35$, and chain lengths ranging from $N = 32$ to 1024 with fixed boundary conditions. The equations of motion have been integrated with a 4th-order Runge-Kutta algorithm and a time step $\Delta t = 0.01$. The results, reported in Fig. 1 clearly reveal a convergence to a κ-value approximately equal to 7 (see the circles). The dotted line represents the best data fit with the function $a + b/N$: the agreement is very good, showing that finite-size corrections to κ are of the order $O(1/N)$, as it should be expected because of the thermal contacts. However, more important than the numerical value of the conductivity is its finiteness in spite of the momentum conservation.

In order to test independently the correctness of our results, we have performed direct microcanonical simulations, which allow determining the thermal conductivity through the Green-Kubo formula [18]:

$$\kappa = \frac{1}{T^2}\int_0^\infty C_J(t)dt \qquad (3)$$

where $C_J(t) = N\langle J(t)J(0)\rangle$ is the flux autocorrelation function at equilibrium and T is the temperature. A correct application of the above formula requires fixing the energy density ε in such a way that the kinetic temperature (defined as $T = \langle p^2\rangle$, in agreement with the virial theorem) is close to the average value of the temperature in the previous simulations. The choice $\varepsilon = 0.5$ turns out to be reasonable, as it corresponds to $T \approx 0.46$. In the absence of thermal baths, the equations of motion are symplectic, so that we have now preferred to use a 6th order McLachlan-Atela integration scheme [19] (with periodic boundary conditions).

The correlation function has been computed by exploiting the Wiener-Khinchin theorem, i.e. by anti-transforming the Fourier power spectrum. The result of the time integration is almost independent of N for $N > 128$. The gray region in Fig. 1 corresponds to the expected value of κ taking into account statistical fluctuations. There is not only a clear confirmation of a finite conductivity, but the numerical value obtained with this technique is in close agreement with the direct estimates.

C. Dynamics in the mode space In order to clarify the difference between the dynamics of the present model and that of FPU-type systems, we have investigated the evolution of the low-frequency Fourier modes. In Fig. 2 we have reported the power spectra of some long-wavelength modes. For the sake of comparison, the same quantities are reported for a diatomic FPU-chain, that is characterized by an anomalous transport. At variance with the FPU model, in the rotators there is no sharp peak (which is a signal of an effective propagation of correlations [9]). Quite differently, the low-frequency part of the spectrum is described very well by a Lorentzian with halfwidth $\gamma = Dk^2$ ($D \approx 4.3$). This represents an independent proof that energy diffuses, as one expects whenever the Fourier law is established.

D. Temperature dependence of the thermal conductivity The most natural question arising from these results concerns the reason for the striking difference with other symmetric models such as the FPU-β system. As long as each $(q_{i+1} - q_i)$ remains confined to the same valley of the potential, there cannot be any qualitative difference with the models previously studied in the literature. Jumps thorugh the barrier, however, appear to act as localized random kicks that contribute to scattering the low-frequency modes and thus to a finite conductivity. If this intuition is correct, one should find analogies between the temperature dependence of the conductivity and the average escape time from the potential well. To this aim, we have computed κ for different temperature values by performing microcanonical simulations with various energy densities. From the data reported in Fig. 3, one can notice a divergence for $T \to 0$ of the type $\kappa \approx \exp(\alpha/T)$ with $\alpha \approx 1.2$. An even more convincing evidence of this behavior is provided by the temperature dependence of the average escape time (see the triangles

in Fig. 3) with an exponent $\alpha \approx 2$. The latter behaviour can be explained by assuming that the jumps are the results of activation processes. Accordingly, the probability of their occurrence is proportional to $\exp(-\Delta V/T)$, where ΔV is the barrier height and the Boltzmann constant is fixed equal to 1 (as implicitely done throughout the Letter). Since $\Delta V = 2$, the whole interpretation is consistent. Moreover, in the absence of jumps, the dependence of the conductivity on the length should be the same as in FPU-systems, i.e. $\kappa \approx N^{2/5}$. Therefore, a low-frequency mode travelling along the chain should experience a conductivity of the order of $\overline{N}^{2/5}$, where $\overline{N}$ is the average separation between jumps. Under the assumption of a uniform distribution of phase jumps, their spatial separation is of the same order of their time separation, so that we can expect that $\kappa \approx \exp[2\Delta V/(5T)]$. On the one hand, this heuristic argument explains why and how such jumps contribute to a normal transport. On the other hand, the numerical disagreement between the observed and the expected value of the exponent α (1.2 vs. 0.8) indicates that our analysis needs refinements. In fact, we should, e.g., notice that, in the low-energy limit, nonlinearities become negligible, implying that deviations from the asymptotic law $\kappa \approx N^{2/5}$ should become relevant.

E. Further checks In order to test the conjecture that jumps are responsible for a normal heat transport, we have decided to investigate some other models. First, we have considered a double-well potential $V(x) = -x^2/2 + x^4/4$ (the same as in FPU with a different sign for the harmonic term). The results of the direct simulations are reported in Fig.1 (see triangles) for a temperature corresponding again to a quarter of the barrier height. The finiteness of the conductivity ans its numerical value is confirmed by the computation of κ through the Green-Kubo formula (see the light-grey shaded region).

Finally, we have considered an asymmetric version of the rotator model, namely $V(x) = A - \cos(x) + 0.4\sin(2x)$, where A is fixed in such a way that the minimum of the potential energy is zero, and the temperature again corresponds to one quarter of the barrier height. In this case too, the conductivity is finite, confirming our empirical idea that the jumps are responsible for breaking the coherence of the energy flux and, in turn, for the finite conductivity. However, from the point of view of Ref. [12], this result is quite unexpected, since, in view of the model asymmetry, one expects that the pressure $\phi = \langle \sum f_i \rangle / N$ is non-zero. Nonetheless, microcanonical simulations show that although the distribution of forces is definitely asymmetric, their average value is numerically 0. This can be understood by noticing that in view of the boundedness of the potential, the system cannot sustain any compression. Therefore, no contradiction exists with Ref. [12].

In conclusion, in this Letter we have reported about the first evidence of normal heat transport in 1d systems with momentum conservation. Such a behaviour appears to be connected with jumps between neighbouring potential valleys. From the dynamical point of view, it is natural to ask what are the peculiar properties of such jumps that make them so different from other types of nonlinear fluctuations that may occur in single-well type of potentials. The only clearly distinctive feature that we have found is the "hyperbolic" type of behaviour in the vicinity of a maximum of the potential which has to be confronted with the typical "ellyptic" character of the oscillations around the minima. We hope to be able to understand in the future whether this is truly the reason for the difference in FPU and rotator systems.

We thank S. Lepri for several profitable discussions. One of us (AP) thanks Gat Omri for some remarks about our last comments. ISI in Torino is acknowledged for the kind hospitality during the Workshop on "Complexity and Chaos" 1998, where part of this work was performed.

[1] Z. Rieder, J.L. Lebowitz, and E. Lieb, J. Math. Phys. **8**, 1073 (1967).
[2] J. B. Keller, G. C. Papanicolau, J. Weilenmann, Comm. Pure and Appl. Math., Vol. XXXII, 583 (1978)
[3] Throughout the paper we shall always assume $m_i = 1$ unless otherwise stated.
[4] G. Casati, J. Ford, F. Vivaldi, W. M. Visscher, Phys. Rev. Lett. **52** 1861 (1984).
[5] T. Prosen, M. Robnik, J. Phys. A **25**, 3449 (1992)
[6] S. Lepri, R. Livi, A. Politi, Phys. Rev. Lett. **78**, 1896 (1997); Physica D, **119**, 140 (1998).
[7] The lattice spacing is assumed equal to 1 without loss of generality.
[8] Y. Pomeau, R. Résibois, Phys. Rep. **19** 63 (1975).
[9] S. Lepri, R. Livi, A. Politi, Europhys. Letters **43**, 271 (1998).
[10] T. Hatano, Phys. Rev. E. **59**, 1 (1999); M. Vassalli, Diploma Thesis, University of Florence, Italy (1999).
[11] B. Hu, B.-W. Li, and H. Zhao. Phys. Rev. E **57**, 2992 (1998).
[12] T. Prosen and D.K. Campbell, chao-dyn/990821/
[13] G. Benettin, L. Galgani and A. Giorgilli, *Il Nuovo Cimento* **B89**, 89 (1985).
[14] R. Livi, M. Pettini, S. Ruffo, A. Vulpiani *J. Stat. Phys.* **48** 539 (1987); D. Escande, H.Kantz, R.Livi, S.Ruffo *J. Stat. Phys.* **76** 605 (1994)
[15] L. Casetti, C. Clementi, and M. Pettini, Phys. Rev. E **54** 5969 (1996)
[16] S. Nosé, J. Chem. Phys. **81** 511 (1984); W. G. Hoover Phys. Rev. A **31** 1695 (1985)
[17] Ph. Choquard, Helvetica Phisica Acta, bf 36 415 (1963)
[18] R. Kubo, M. Toda, N. Hashitsume, *Statistical Physics II*, Springer Series in Solid State Sciences, Vol. 31 (1991)
[19] R.I. Mclachlan, P. Atela, Nonlinearity **5**, 541 (1992).

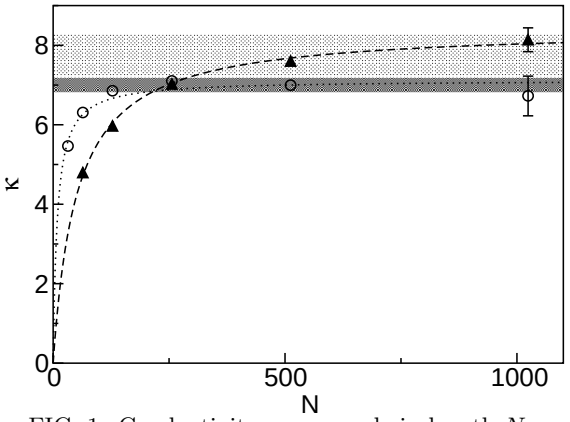

Fig. 1 Giardina' et al.

FIG. 1. Conductivity κ versus chain length N as obtained from non-equilibrium molecular dynamics. Circles correspond to the rotator model with temperatures $T_L = 0.55$ and $T_R = 0.35$; triangles correspond to the double well potential with $T_L = 0.04$ and $T_R = 0.06$. The two lines represent the best fit with the function $a+b/N$. The two shaded regions represent the uncertainty about the conductivity on the basis of the Green-Kubo formula.

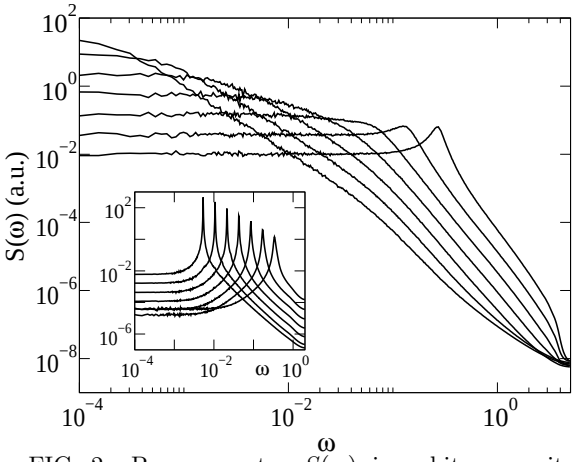

Fig. 2 Giardina' et al.

FIG. 2. Power spectra $S(w)$ in arbitrary units of the Fourier modes 1,2,4,8,16,32 and 64 (curves from left to right in the high frequency 'region) in a chain of length $N = 1024$ of rotators with energy density with energy density 0.5. The curves result from an average over 1000 independent initial conditions. In the inset, the same modes are reported for a diatomic FPU chain with masses 1, 2 and energy density 8.8.

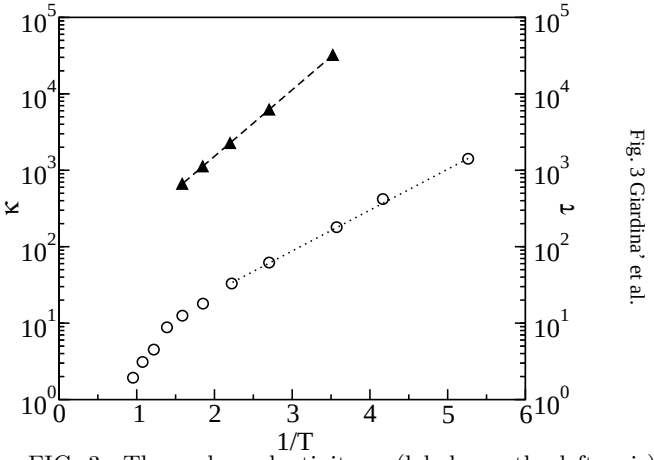

Fig. 3 Giardina' et al.

FIG. 3. Thermal conductivity κ (labels on the left axis) versus the inverse temperature $1/T$ in the rotator model (open circles). Triangles correspond to the average time separation between consecutive phase jumps (labels on the right axis) in the same system.